



ELSEVIER

Chemical Physics 271 (2001) 369–372

Chemical  
Physics

www.elsevier.com/locate/chemphys

## Author Index

- Amat-Guerri, F., see Bergmann, A. 271 (2001) 201
- Bae, Y.C., see Yoon, D.K. 271 (2001) 183
- Bencivenni, L., see Ramondo, F. 271 (2001) 293
- Benderskii, V.A., E.V. Vetoshkin and H.P. Trommsdorff, Tunneling splittings in vibrational spectra of non-rigid molecules. X. Reaction path Hamiltonian as zero-order approximation 271 (2001) 165
- Bergmann, A., W. Holzer, R. Stark, H. Gratz, A. Penzkofer, F. Amat-Guerri, A. Costela, I. Garcia-Moreno and R. Sastre, Photophysical characterization of pyromethene dyes in solid matrices of acrylic copolymers 271 (2001) 201
- Białkowska-Jaworska, E., see Milet, A. 271 (2001) 267
- Biskupič, S., see Lukeš, V. 271 (2001) 1
- Bodo, E., F.A. Gianturco, R. Martinazzo and M. Raimondi, Possible reaction paths in the  $\text{LiH}_2^+$  chemistry: a computational analysis of the interaction forces 271 (2001) 309
- Bu, Y., C. Xiahou and X. Song, The structural character of  $\text{AlS}_2$  species in quartet state: prediction at density functional theory and the correlated-wave function levels 271 (2001) 229
- Caputo, R., A.V. Sukhov, N.V. Tabirian, C. Umeton and R.F. Ushakov, Mass transfer processes induced by inhomogeneous photo-polymerisation in a multicomponent medium 271 (2001) 323
- Castano, F., see Unamuno, I. 271 (2001) 55
- Chang, Ch., A.B.C. Patzer, E. Sedlmayr, T. Steinke and D. Sülzle, A density functional study of small  $(\text{AlN})_n$  clusters: structures, energies, and frequencies 271 (2001) 283
- Chesnut, D.B., The use of parameter ratios to characterize the formal order of chemical bonds 271 (2001) 9
- Costela, A., see Bergmann, A. 271 (2001) 201
- Dai, D., see Dai, Y. 271 (2001) 71
- Dai, Y., D. Dai and S.-l. Ding, Study on multiphoton processes in intense laser fields using the quadratic anharmonic Lie algebraic hamiltonian of diatomic molecule 271 (2001) 71
- Del Zoppo, M., see Sugliani, S. 271 (2001) 127
- Deleuze, M.S., see Salam, A. 271 (2001) 17
- Ding, S.-l., see Dai, Y. 271 (2001) 71
- Diósi, L., see Wiseman, H.M. 271 (2001) 227

- Fernández, J.A., see Unamuno, I. 271 (2001) 55  
François, J.-P., see Salam, A. 271 (2001) 17
- García-Moreno, I., see Bergmann, A. 271 (2001) 201  
Gianturco, F.A., see Bodo, E. 271 (2001) 309  
Gontrani, L., see Ramondo, F. 271 (2001) 293  
Gratz, H., see Bergmann, A. 271 (2001) 201
- Herman, M., see Mellouki, A. 271 (2001) 239  
Holland, D.M.P., see Potts, A.W. 271 (2001) 337  
Holzer, W., see Bergmann, A. 271 (2001) 201
- Jen, A.K.-Y., see Woodford, J.N. 271 (2001) 137
- Karlsson, L., see Potts, A.W. 271 (2001) 337  
Kato, T., M. Kondo, M. Tachibana, T. Yamabe and K. Yoshizawa, Vibronic interaction in a copper oxide cluster 271 (2001) 31  
Kisiel, Z., see Milet, A. 271 (2001) 267  
Kondo, M., see Kato, T. 271 (2001) 31
- Landajo, C., see Unamuno, I. 271 (2001) 55  
Laurinc, V., see Lukeš, V. 271 (2001) 1  
Liévin, J., see Mellouki, A. 271 (2001) 239  
Lokhman, V.N., D.D. Ogurok and E.A. Ryabov, Photoionization detection of CF<sub>2</sub> radicals resulting from the IR multiple-photon dissociation of CF<sub>2</sub>HCl molecules in a molecular beam 271 (2001) 357  
Longarte, A., see Unamuno, I. 271 (2001) 55  
Lukeš, V., I. Vrabel, V. Laurinc and S. Biskupič, Ab initio study of the Li(<sup>2</sup>S)-H<sub>2</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) van der Waals complex 271 (2001) 1
- Mahapatra, S., see Ritschel, T. 271 (2001) 155  
Makarov, V.I., Magnetic field effect on the H<sub>2</sub>CS fluorescence from the first excited singlet state  $\tilde{A}^1A_2$  271 (2001) 79  
Makshantsev, B.I. and V.B. Makshantsev, On the photon vector potential 271 (2001) 97  
Makshantsev, B.I. and V.B. Makshantsev, On scattering cross sections of the photons' ensemble 271 (2001) 107  
Makshantsev, V.B., see Makshantsev, B.I. 271 (2001) 97  
Makshantsev, V.B., see Makshantsev, B.I. 271 (2001) 107  
Martinazzo, R., see Bodo, E. 271 (2001) 309  
Mellouki, A., J. Liévin and M. Herman, The vibrational spectrum of pyrrole (C<sub>4</sub>H<sub>5</sub>N) and furan (C<sub>4</sub>H<sub>4</sub>O) in the gas phase 271 (2001) 239  
Milet, A., C. Struniewicz, R. Moszynski, J. Sadlej, Z. Kisiel, E. Białkowska-Jaworska and L. Pszczółkowski, Structure and properties of the weakly bound trimer (H<sub>2</sub>O)<sub>2</sub>HCl. Theoretical predictions and comparison with high-resolution rotational spectroscopy 271 (2001) 267  
Moszynski, R., see Milet, A. 271 (2001) 267  
Müller, A., see Renge, I. 271 (2001) 191  
Mutoh, H., see Ogi, Y. 271 (2001) 215

- Ogi, Y., A. Sakoda, H. Mutoh, H. Taki and K. Tsukiyama, Polarization properties of laser induced amplified spontaneous emission from NO Rydberg states 271 (2001) 215
- Ogurok, D.D., see Likhman, V.N. 271 (2001) 357
- Patzer, A.B.C., see Chang, Ch. 271 (2001) 283
- Penzkofer, A., see Bergmann, A. 271 (2001) 201
- Pieretti, A., see Ramondo, F. 271 (2001) 293
- Potts, A.W., A.B. Trofimov, J. Schirmer, D.M.P. Holland and L. Karlsson, An experimental and theoretical study of the valence shell photoelectron spectra of 2-bromothiophene and 3-bromothiophene 271 (2001) 337
- Pszczólkowski, L., see Milet, A. 271 (2001) 267
- Raimondi, M., see Bodo, E. 271 (2001) 309
- Ramondo, F., A. Pieretti, L. Gontrani and L. Bencivenni, Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study 271 (2001) 293
- Renge, I., A. Müller and U.P. Wild, High resolution spectroscopy of a hydrocarbon with the triplet ground state, 2,2-dimethyl-2H-dibenzo[cd,k]fluoranthene and its closed-shell precursor in solid matrices 271 (2001) 191
- Ritschel, T., S. Mahapatra and L. Zülke, Quasiclassical dynamics of proton scattering by N<sub>2</sub>( $\Sigma_g^+$ ) on an improved ab initio potential energy surface 271 (2001) 155
- Ryabov, E.A., see Likhman, V.N. 271 (2001) 357
- Sadlej, J., see Milet, A. 271 (2001) 267
- Sakoda, A., see Ogi, Y. 271 (2001) 215
- Salam, A., M.S. Deleuze and J.-P. François, Ab initio and density functional theory calculation of the structure and vibrational properties of *n*-vertex *clos*o-carboranes, *n* = 5, 6 and 7 271 (2001) 17
- Sastre, R., see Bergmann, A. 271 (2001) 201
- Schirmer, J., see Potts, A.W. 271 (2001) 337
- Sedlmayr, E., see Chang, Ch. 271 (2001) 283
- Shu, C.-F., see Sugliani, S. 271 (2001) 127
- Song, X., see Bu, Y. 271 (2001) 229
- Stark, R., see Bergmann, A. 271 (2001) 201
- Stavrov, S.S., Optical absorption band III of deoxyheme proteins as a probe of their structure and dynamics 271 (2001) 145
- Steinke, T., see Chang, Ch. 271 (2001) 283
- Struniewicz, C., see Milet, A. 271 (2001) 267
- Sugliani, S., M. Del Zoppo, G. Zerbi and C.-F. Shu, Chain flexibility and nonlinear optical properties in polyenes within a two-state (VB-CT) model 271 (2001) 127
- Sukhov, A.V., see Caputo, R. 271 (2001) 323
- Sülzle, D., see Chang, Ch. 271 (2001) 283
- Suzuki, A., see Yoshizawa, K. 271 (2001) 41
- Tabirian, N.V., see Caputo, R. 271 (2001) 323
- Tachibana, M., see Kato, T. 271 (2001) 31
- Taki, H., see Ogi, Y. 271 (2001) 215
- Trofimov, A.B., see Potts, A.W. 271 (2001) 337

- Trommsdorff, H.P., see Benderskii, V.A. 271 (2001) 165  
Tsukiyama, K., see Ogi, Y. 271 (2001) 215
- Umeton, C., see Caputo, R. 271 (2001) 323
- Unamuno, I., J.A. Fernández, C. Landajo, A. Longarte and F. Castaño, Binding energy and structure of the ground, first electronic and ion states of *p*-methoxyphenethylamine( $H_2O$ )<sub>1</sub> isomers: a combined experimental and theoretical study 271 (2001) 55  
Ushakov, R.F., see Caputo, R. 271 (2001) 323
- Vetoshkin, E.V., see Benderskii, V.A. 271 (2001) 165  
Vrábel, I., see Lukeš, V. 271 (2001) 1
- Wang, C.H., see Woodford, J.N. 271 (2001) 137  
Wild, U.P., see Renge, I. 271 (2001) 191  
Wiseman, H.M. and L. Diósi, Erratum to "Complete parameterization, and invariance, of diffusive quantum trajectories for Markovian open systems" [Chem. Phys. 268 (2001) 91–104] 271 (2001) 227  
Woodford, J.N., C.H. Wang and A.K.-Y. Jen, Dispersion of the first molecular hyperpolarizability of charge-transfer chromophores studied by hyper-Rayleigh scattering 271 (2001) 137
- Xiahou, C., see Bu, Y. 271 (2001) 229
- Yamabe, T., see Kato, T. 271 (2001) 31  
Yoon, D.K. and Y.C. Bae, Phase behaviors of smectic-A liquid crystal/linear polymer systems 271 (2001) 183  
Yoshizawa, K. and A. Suzuki, Configurational inversion of the tetrahedral molecules  $CH_4$ ,  $SiH_4$ , and  $GeH_4$  271 (2001) 41  
Yoshizawa, K., see Kato, T. 271 (2001) 31
- Zerbi, G., see Sugliani, S. 271 (2001) 127  
Zülicke, L., see Ritschel, T. 271 (2001) 155

## Subject Index

### Methods and constructs

#### Theoretical

##### *Computational methods for electronic structure*

- The use of parameter ratios to characterize the formal order of chemical bonds, D.B. Chesnut 271 (2001) 9
- Ab initio and density functional theory calculation of the structure and vibrational properties of *n*-vertex *closo*-carboranes, *n* = 5, 6 and 7, A. Salam, M.S. Deleuze and J.-P. François 271 (2001) 17
- The structural character of  $\text{AlS}_2$  species in quartet state: prediction at density functional theory and the correlated-wave function levels, Y. Bu, C. Xiahou and X. Song 271 (2001) 229
- The vibrational spectrum of pyrrole ( $\text{C}_4\text{H}_5\text{N}$ ) and furan ( $\text{C}_4\text{H}_4\text{O}$ ) in the gas phase, A. Mellouki, J. Liévin and M. Herman 271 (2001) 239

##### *-perturbative and many body approaches*

- Ab initio study of the  $\text{Li}(\text{}^2\text{S})-\text{H}_2(\text{X}^1\Sigma_g^+)$  van der Waals complex, V. Lukeš, I. Vrábel, V. Laurinc and S. Biskupič 271 (2001) 1
- Structure and properties of the weakly bound trimer  $(\text{H}_2\text{O})_2\text{HCl}$ . Theoretical predictions and comparison with high-resolution rotational spectroscopy, A. Milet, C. Struniewicz, R. Moszynski, J. Sadlej, Z. Kisiel, E. Białkowska-Jaworska and L. Pszczółkowski 271 (2001) 267

##### *-density functional theory*

- The use of parameter ratios to characterize the formal order of chemical bonds, D.B. Chesnut 271 (2001) 9
- Ab initio and density functional theory calculation of the structure and vibrational properties of *n*-vertex *closo*-carboranes, *n* = 5, 6 and 7, A. Salam, M.S. Deleuze and J.-P. François 271 (2001) 17
- Vibronic interaction in a copper oxide cluster, T. Kato, M. Kondo, M. Tachibana, T. Yamabe and K. Yoshizawa 271 (2001) 31
- Configurational inversion of the tetrahedral molecules  $\text{CH}_4$ ,  $\text{SiH}_4$ , and  $\text{GeH}_4$ , K. Yoshizawa and A. Suzuki 271 (2001) 41

- Binding energy and structure of the ground, first electronic and ion states of *p*-methoxyphenethylamine( $\text{H}_2\text{O}$ )<sub>1</sub> isomers: a combined experimental and theoretical study, I. Unamuno, J.A. Fernández, C. Landajo, A. Longarte and F. Castaño 271 (2001) 55
- A density functional study of small  $(\text{AlN})_x$  clusters: structures, energies, and frequencies, Ch. Chang, A.B.C. Patzer, E. Sedlmayr, T. Steinke and D. Sülzle 271 (2001) 283
- Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study, F. Ramondo, A. Pieretti, L. Gontrani and L. Bencivenni 271 (2001) 293
- Algebraic approaches*
- Study on multiphoton processes in intense laser fields using the quadratic anharmonic Lie algebraic hamiltonian of diatomic molecule, Y. Dai, D. Dai, and S.-l. Ding 271 (2001) 71
- Spin states and magnetic interactions*
- Magnetic field effect on the  $\text{H}_2\text{CS}$  fluorescence from the first excited singlet state  $\tilde{\text{A}}^1\text{A}_2$ , V.I. Makarov 271 (2001) 79
- Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)*
- On the photon vector potential, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 97
- On scattering croasses of the photons' ensemble, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 107
- Chain flexibility and nonlinear optical properties in polyenes within a two-state (VB-CT) model, S. Sugliani, M. Del Zoppo, G. Zerbi and C.-F. Shu 271 (2001) 127
- Dispersion of the first molecular hyperpolarizability of charge-transfer chromophores studied by hyper-Rayleigh scattering, J.N. Woodford, C.H. Wang and A.K.-Y. Jen 271 (2001) 137
- Radiative (incl. relativistic) effects on molecules and molecular processes*
- On the photon vector potential, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 97
- On scattering croasses of the photons' ensemble, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 107
- Optical absorption band III of deoxyheme proteins as a probe of their structure and dynamics, S.S. Stavrov 271 (2001) 145
- Scattering of waves and particles*
- On the photon vector potential, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 97
- On scattering croasses of the photons' ensemble, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 107
- Collisional and reactive molecular dynamics with non-frictional forces*
- Quasiclassical dynamics of proton scattering by  $\text{N}_2(^1\Sigma_g^+)$  on an improved ab initio potential energy surface, T. Ritschel, S. Mahapatra and L. Zülicke 271 (2001) 155
- Intramolecular dynamics*
- Tunneling splittings in vibrational spectra of non-rigid molecules. X. Reaction path Hamiltonian as zero-order approximation, V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff 271 (2001) 165
- Molecular dynamics of many particle systems and condensed phases*
- Possible reaction paths in the  $\text{LiH}_2^+$  chemistry: a computational analysis of the interaction forces, E. Bodo, F.A. Gianturco, R. Martinazzo and M. Raimondi 271 (2001) 309



- Mass transfer processes induced by inhomogeneous photo-polymerisation in a multicomponent medium, R. Caputo, A.V. Sukhov, N.V. Tabirian, C. Umeton and R.F. Ushakov 271 (2001) 323

*Equilibrium statistical mechanics and thermodynamics*

- Phase behaviors of smectic-A liquid crystal/linear polymer systems, D.K. Yoon and Y.C. Bae 271 (2001) 183

**Experiment**

*Molecular spectroscopy*

- Binding energy and structure of the ground, first electronic and ion states of *p*-methoxyphenethylamine( $\text{H}_2\text{O}$ )<sub>1</sub> isomers: a combined experimental and theoretical study, I. Unamuno, J.A. Fernández, C. Landajo, A. Longarte and F. Castaño 271 (2001) 55

*-microwave*

- Structure and properties of the weakly bound trimer ( $\text{H}_2\text{O}$ )<sub>2</sub>HCl. Theoretical predictions and comparison with high-resolution rotational spectroscopy, A. Milet, C. Struniewicz, R. Moszynski, J. Sadlej, Z. Kisiel, E. Białkowska-Jaworska and L. Pszczółkowski 271 (2001) 267

*-infrared*

- Chain flexibility and nonlinear optical properties in polyenes within a two-state (VB-CT) model, S. Sugliani, M. Del Zoppo, G. Zerbi and C.-F. Shu 271 (2001) 127
- Optical absorption band III of deoxyheme proteins as a probe of their structure and dynamics, S.S. Stavrov 271 (2001) 145
- The vibrational spectrum of pyrrole ( $\text{C}_4\text{H}_5\text{N}$ ) and furan ( $\text{C}_4\text{H}_4\text{O}$ ) in the gas phase, A. Mellouki, J. Liévin and M. Herman 271 (2001) 239
- Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study, F. Ramondo, A. Pieretti, L. Gontrani and L. Bencivenni 271 (2001) 293

*-Raman*

- Chain flexibility and nonlinear optical properties in polyenes within a two-state (VB-CT) model, S. Sugliani, M. Del Zoppo, G. Zerbi and C.-F. Shu 271 (2001) 127

*-visible*

- High resolution spectroscopy of a hydrocarbon with the triplet ground state, 2,2-dimethyl-2*H*-dibenzo[*cd,k*]fluoranthene and its closed-shell precursor in solid matrices, I. Renge, A. Müller and U.P. Wild 271 (2001) 191

*Photoelectron and Auger spectroscopy*

- An experimental and theoretical study of the valence shell photoelectron spectra of 2-bromothiophene and 3-bromothiophene, A.W. Potts, A.B. Trofimov, J. Schirmer, D.M.P. Holland and L. Karlsson 271 (2001) 337

*Multiphoton ionization*

- Photoionization detection of  $\text{CF}_2$  radicals resulting from the IR multiple-photon dissociation of  $\text{CF}_2\text{HCl}$  molecules in a molecular beam, V.N. Likhman, D.D. Ogurok and E.A. Ryabov 271 (2001) 357

*Laser induced fluorescence*

- Magnetic field effect on the  $\text{H}_2\text{CS}$  fluorescence from the first excited singlet state  $\tilde{\text{A}}^1\text{A}_2$ , V.I. Makarov 271 (2001) 79
- Photophysical characterization of pyrromethene dyes in solid matrices of acrylic copolymers, A. Bergmann, W. Holzer, R. Stark, H. Gratz, A. Penzkofer, F. Amat-Guerri, A. Costela, I. García-Moreno and R. Sastre 271 (2001) 201
- Polarization properties of laser induced amplified spontaneous emission from NO Rydberg states, Y. Ogi, A. Sakoda, H. Mutoh, H. Taki and K. Tsukiyama 271 (2001) 215

*Ultrafast measurements*

- Photophysical characterization of pyrromethene dyes in solid matrices of acrylic copolymers, A. Bergmann, W. Holzer, R. Stark, H. Gratz, A. Penzkofer, F. Amat-Guerri, A. Costela, I. García-Moreno and R. Sastre 271 (2001) 201

*Nonlinear optics and spectroscopy*

- Dispersion of the first molecular hyperpolarizability of charge-transfer chromophores studied by hyper-Rayleigh scattering, J.N. Woodford, C.H. Wang and A.K.-Y. Jen 271 (2001) 137
- Polarization properties of laser induced amplified spontaneous emission from NO Rydberg states, Y. Ogi, A. Sakoda, H. Mutoh, H. Taki and K. Tsukiyama 271 (2001) 215

*Synchrotron spectroscopies*

- An experimental and theoretical study of the valence shell photoelectron spectra of 2-bromothiophene and 3-bromothiophene, A.W. Potts, A.B. Trofimov, J. Schirmer, D.M.P. Holland and L. Karlsson 271 (2001) 337

*Multiple resonance spectroscopy*

- Polarization properties of laser induced amplified spontaneous emission from NO Rydberg states, Y. Ogi, A. Sakoda, H. Mutoh, H. Taki and K. Tsukiyama 271 (2001) 215

*Measurement of macroscopic variables*

- Phase behaviors of smectic-A liquid crystal/linear polymer systems, D.K. Yoon and Y.C. Bae 271 (2001) 183
- Mass transfer processes induced by inhomogeneous photo-polymerisation in a multicomponent medium, R. Caputo, A.V. Sukhov, N.V. Tabirian, C. Umeton and R.F. Ushakov 271 (2001) 323

**Objects****Bulk systems***Gases*

- Magnetic field effect on the  $\text{H}_2\text{CS}$  fluorescence from the first excited singlet state  $\tilde{\text{A}}^1\text{A}_2$ , V.I. Makarov 271 (2001) 79
- Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study, F. Ramondo, A. Pieretti, L. Gontrani and L. Bencivenni 271 (2001) 293



- Possible reaction paths in the  $\text{LiH}_2^+$  chemistry: a computational analysis of the interaction forces, E. Bodo, F.A. Gianturco, R. Martinazzo and M. Raimondi 271 (2001) 309
- Supersonic beams*
- Binding energy and structure of the ground, first electronic and ion states of *p*-methoxyphenethylamine( $\text{H}_2\text{O}$ )<sub>1</sub> isomers: a combined experimental and theoretical study, I. Unamuno, J.A. Fernández, C. Landajo, A. Longarte and F. Castaño 271 (2001) 55
- Photoionization detection of  $\text{CF}_2$  radicals resulting from the IR multiple-photon dissociation of  $\text{CF}_2\text{HCl}$  molecules in a molecular beam, V.N. Lokhman, D.D. Ogurok and E.A. Ryabov 271 (2001) 357
- Liquid mixtures and solutions*
- Dispersion of the first molecular hyperpolarizability of charge-transfer chromophores studied by hyper-Rayleigh scattering, J.N. Woodford, C.H. Wang and A.K.-Y. Jen 271 (2001) 137
- Glasses*
- High resolution spectroscopy of a hydrocarbon with the triplet ground state, 2,2-dimethyl-2H-dibenzo[*cd,k*]fluoranthene and its closed-shell precursor in solid matrices, I. Renge, A. Müller and U.P. Wild 271 (2001) 191
- Complex fluids*
- liquid crystals*
- Phase behaviors of smectic-A liquid crystal/linear polymer systems, D.K. Yoon and Y.C. Bae 271 (2001) 183
- Mass transfer processes induced by inhomogeneous photo-polymerisation in a multicomponent medium, R. Caputo, A.V. Sukhov, N.V. Tabirian, C. Umeton and R.F. Ushakov 271 (2001) 323
- Semiconductors*
- Vibronic interaction in a copper oxide cluster, T. Kato, M. Kondo, M. Tachibana, T. Yamabe and K. Yoshizawa 271 (2001) 31
- Microscopic and mesoscopic systems**
- Single atoms, molecules and assemblies (incl. biological)*
- The use of parameter ratios to characterize the formal order of chemical bonds, D.B. Chesnut 271 (2001) 9
- Study on multiphoton processes in intense laser fields using the quadratic anharmonic Lie algebraic hamiltonian of diatomic molecule, Y. Dai, D. Dai and S.-l. Ding 271 (2001) 71
- Molecules (neutral and ionic)*
- Quasiclassical dynamics of proton scattering by  $\text{N}_2(^1\Sigma_g^+)$  on an improved ab initio potential energy surface, T. Ritschel, S. Mahapatra and L. Zülicke 271 (2001) 155
- diatomic*
- Polarization properties of laser induced amplified spontaneous emission from NO Rydberg states, Y. Ogi, A. Sakoda, H. Mutoh, H. Taki and K. Tsukiyama 271 (2001) 215

- Possible reaction paths in the  $\text{LiH}_2^+$  chemistry: a computational analysis of the interaction forces, E. Bodo, F.A. Gianturco, R. Martinazzo and M. Raimondi 271 (2001) 309
- small polyatomics*
- Configurational inversion of the tetrahedral molecules  $\text{CH}_4$ ,  $\text{SiH}_4$ , and  $\text{GeH}_4$ , K. Yoshizawa and A. Suzuki 271 (2001) 41
- Magnetic field effect on the  $\text{H}_2\text{CS}$  fluorescence from the first excited singlet state  $\tilde{\text{A}}^1\text{A}_2$ , V.I. Makarov 271 (2001) 79
- Tunneling splittings in vibrational spectra of non-rigid molecules. X. Reaction path Hamiltonian as zero-order approximation, V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff 271 (2001) 165
- The structural character of  $\text{AlS}_2$  species in quartet state: prediction at density functional theory and the correlated-wave function levels, Y. Bu, C. Xiahou and X. Song 271 (2001) 229
- Photoionization detection of  $\text{CF}_2$  radicals resulting from the IR multiple-photon dissociation of  $\text{CF}_2\text{HCl}$  molecules in a molecular beam, V.N. Likhman, D.D. Ogurok and E.A. Ryabov 271 (2001) 357
- aromatics*
- Dispersion of the first molecular hyperpolarizability of charge-transfer chromophores studied by hyper-Rayleigh scattering, J.N. Woodford, C.H. Wang and A.K.-Y. Jen 271 (2001) 137
- High resolution spectroscopy of a hydrocarbon with the triplet ground state, 2,2-dimethyl-2H-dibenzo[cd,k]fluoranthene and its closed-shell precursor in solid matrices, I. Renge, A. Müller and U.P. Wild 271 (2001) 191
- Photophysical characterization of pyrromethene dyes in solid matrices of acrylic copolymers, A. Bergmann, W. Holzer, R. Stark, H. Gratz, A. Penzkofer, F. Amat-Guerri, A. Costela, I. García-Moreno and R. Sastre 271 (2001) 201
- The vibrational spectrum of pyrrole ( $\text{C}_4\text{H}_5\text{N}$ ) and furan ( $\text{C}_4\text{H}_4\text{O}$ ) in the gas phase, A. Mellouki, J. Liévin and M. Herman 271 (2001) 239
- An experimental and theoretical study of the valence shell photoelectron spectra of 2-bromothiophene and 3-bromothiophene, A.W. Potts, A.B. Trofimov, J. Schirmer, D.M.P. Holland and L. Karlsson 271 (2001) 337
- other large*
- Chain flexibility and nonlinear optical properties in polyenes within a two-state (VB-CT) model, S. Sugliani, M. Del Zoppo, G. Zerbi and C.-F. Shu 271 (2001) 127
- Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study, F. Ramondo, A. Pieretti, L. Gontrani and L. Bencivenni 271 (2001) 293
- polymeric and biological*
- Phase behaviors of smectic-A liquid crystal/linear polymer systems, D.K. Yoon and Y.C. Bae 271 (2001) 183
- Molecular aggregates*
- Ab initio and density functional theory calculation of the structure and vibrational properties of  $n$ -vertex *closo*-carboranes,  $n = 5, 6$  and  $7$ , A. Salam, M.S. Deleuze and J.-P. François 271 (2001) 17

- Binding energy and structure of the ground, first electronic and ion states of *p*-methoxyphenethylamine( $\text{H}_2\text{O}$ )<sub>1</sub> isomers: a combined experimental and theoretical study, I. Unamuno, J.A. Fernández, C. Landajo, A. Longarte and F. Castaño 271 (2001) 55
- A density functional study of small  $(\text{AlN})_x$  clusters: structures, energies, and frequencies, Ch. Chang, A.B.C. Patzer, E. Sedlmayr, T. Steinke and D. Sülzle 271 (2001) 283
- dimers*
- Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study, F. Ramondo, A. Pieretti, L. Gontrani and L. Bencivenni 271 (2001) 293
- van der Waals molecules*
- Ab initio study of the  $\text{Li}(^2\text{S})-\text{H}_2(\text{X}^1\Sigma_g^+)$  van der Waals complex, V. Lukeš, I. Vrábel, V. Laurinc and S. Biskupić 271 (2001) 1
- clusters*
- Ab initio and density functional theory calculation of the structure and vibrational properties of *n*-vertex *closo*-carboranes,  $n = 5, 6$  and  $7$ , A. Salam, M.S. Deleuze and J.-P. François 271 (2001) 17
- Structure and properties of the weakly bound trimer  $(\text{H}_2\text{O})_2\text{HCl}$ . Theoretical predictions and comparison with high-resolution rotational spectroscopy, A. Milet, C. Struniewicz, R. Moszynski, J. Sadlej, Z. Kisiel, E. Białkowska-Jaworska and L. Piszczółkowski 271 (2001) 267
- A density functional study of small  $(\text{AlN})_x$  clusters: structures, energies, and frequencies, Ch. Chang, A.B.C. Patzer, E. Sedlmayr, T. Steinke and D. Sülzle 271 (2001) 283
- Free radicals (incl. hydronium and muonium)*
- Photoionization detection of  $\text{CF}_2$  radicals resulting from the IR multiple-photon dissociation of  $\text{CF}_2\text{HCl}$  molecules in a molecular beam, V.N. Lokhman, D.D. Ogurok and E.A. Ryabov 271 (2001) 357
- Proteins*
- Optical absorption band III of deoxyheme proteins as a probe of their structure and dynamics, S.S. Stavrov 271 (2001) 145

## Phenomena

### Molecular structure

- Ab initio study of the  $\text{Li}(^2\text{S})-\text{H}_2(\text{X}^1\Sigma_g^+)$  van der Waals complex, V. Lukeš, I. Vrábel, V. Laurinc and S. Biskupić 271 (2001) 1
- The use of parameter ratios to characterize the formal order of chemical bonds, D.B. Chesnut 271 (2001) 9
- Ab initio and density functional theory calculation of the structure and vibrational properties of *n*-vertex *closo*-carboranes,  $n = 5, 6$  and  $7$ , A. Salam, M.S. Deleuze and J.-P. François 271 (2001) 17
- Configurational inversion of the tetrahedral molecules  $\text{CH}_4$ ,  $\text{SiH}_4$ , and  $\text{GeH}_4$ , K. Yoshizawa and A. Suzuki 271 (2001) 41

- Binding energy and structure of the ground, first electronic and ion states of *p*-methoxyphenethylamine( $\text{H}_2\text{O}$ )<sub>1</sub> isomers: a combined experimental and theoretical study, I. Unamuno, J.A. Fernández, C. Landajo, A. Longarte and F. Castaño 271 (2001) 55
- Magnetic field effect on the  $\text{H}_2\text{CS}$  fluorescence from the first excited singlet state  $\tilde{\text{A}}^1\text{A}_2$ , V.I. Makarov 271 (2001) 79
- The structural character of  $\text{AlS}_2$  species in quartet state: prediction at density functional theory and the correlated-wave function levels, Y. Bu, C. Xiahou and X. Song 271 (2001) 229
- The vibrational spectrum of pyrrole ( $\text{C}_4\text{H}_5\text{N}$ ) and furan ( $\text{C}_4\text{H}_4\text{O}$ ) in the gas phase, A. Mellouki, J. Liévin and M. Herman 271 (2001) 239
- A density functional study of small  $(\text{AlN})_x$  clusters: structures, energies, and frequencies, Ch. Chang, A.B.C. Patzer, E. Sedlmayr, T. Steinke and D. Sülzle 271 (2001) 283
- Vibrations and rotations of molecules*
- The vibrational spectrum of pyrrole ( $\text{C}_4\text{H}_5\text{N}$ ) and furan ( $\text{C}_4\text{H}_4\text{O}$ ) in the gas phase, A. Mellouki, J. Liévin and M. Herman 271 (2001) 239
- Structure and properties of the weakly bound trimer  $(\text{H}_2\text{O})_2\text{HCl}$ . Theoretical predictions and comparison with high-resolution rotational spectroscopy, A. Milet, C. Struniewicz, R. Moszynski, J. Sadlej, Z. Kisiel, E. Białkowska-Jaworska and L. Pászczółkowski 271 (2001) 267
- Electronic structure and states*
- The use of parameter ratios to characterize the formal order of chemical bonds, D.B. Chesnut 271 (2001) 9
- The structural character of  $\text{AlS}_2$  species in quartet state: prediction at density functional theory and the correlated-wave function levels, Y. Bu, C. Xiahou and X. Song 271 (2001) 229
- An experimental and theoretical study of the valence shell photoelectron spectra of 2-bromothiophene and 3-bromothiophene, A.W. Potts, A.B. Trofimov, J. Schirmer, D.M.P. Holland and L. Karlsson 271 (2001) 337
- Electric and magnetic properties*
- Vibronic interaction in a copper oxide cluster, T. Kato, M. Kondo, M. Tachibana, T. Yamabe and K. Yoshizawa 271 (2001) 31
- Molecular interactions*
- Ab initio study of the  $\text{Li}(\text{}^2\text{S})-\text{H}_2(\text{}^1\Sigma_g^+)$  van der Waals complex, V. Lukeš, I. Vrábel, V. Laurinc and S. Biskupič 271 (2001) 1
- Quasiclassical dynamics of proton scattering by  $\text{N}_2(\text{}^1\Sigma_g^+)$  on an improved ab initio potential energy surface, T. Ritschel, S. Mahapatra and L. Zülicke 271 (2001) 155
- High resolution spectroscopy of a hydrocarbon with the triplet ground state, 2,2-dimethyl-2*H*-dibenzo[*cd,k*]fluoranthene and its closed-shell precursor in solid matrices, I. Renge, A. Müller and U.P. Wild 271 (2001) 191
- Structure and properties of the weakly bound trimer  $(\text{H}_2\text{O})_2\text{HCl}$ . Theoretical predictions and comparison with high-resolution rotational spectroscopy, A. Milet, C. Struniewicz, R. Moszynski, J. Sadlej, Z. Kisiel, E. Białkowska-Jaworska and L. Pászczółkowski 271 (2001) 267
- Spectral bandshapes and intensities*
- On the photon vector potential, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 97

- On scattering crosses of the photons' ensemble, B.I. Makshantsev and V.B. Makshantsev 271 (2001) 107
- Optical absorption band III of deoxyheme proteins as a probe of their structure and dynamics, S.S. Stavrov 271 (2001) 145
- Coupling of electronic and nuclear motion*
- Vibronic interaction in a copper oxide cluster, T. Kato, M. Kondo, M. Tachibana, T. Yamabe and K. Yoshizawa 271 (2001) 31
- Possible reaction paths in the  $\text{LiH}_2^+$  chemistry: a computational analysis of the interaction forces, E. Bodo, F.A. Gianturco, R. Martinazzo and M. Raimondi 271 (2001) 309
- Energy transfer processes*
- Quasiclassical dynamics of proton scattering by  $\text{N}_2(^1\Sigma_g^+)$  on an improved ab initio potential energy surface, T. Ritschel, S. Mahapatra and L. Zülicke 271 (2001) 155
- Molecular photophysical processes*
- Photophysical characterization of pyromethene dyes in solid matrices of acrylic copolymers, A. Bergmann, W. Holzer, R. Stark, H. Gratz, A. Penzkofer, F. Amat-Guerri, A. Costela, I. García-Moreno and R. Sastre 271 (2001) 201
- An experimental and theoretical study of the valence shell photoelectron spectra of 2-bromothiophene and 3-bromothiophene, A.W. Potts, A.B. Trofimov, J. Schirmer, D.M.P. Holland and L. Karlsson 271 (2001) 337
- Luminescence spectra, yields and lifetimes*
- High resolution spectroscopy of a hydrocarbon with the triplet ground state, 2,2-dimethyl-2H-dibenzo[cd,k]fluoranthene and its closed-shell precursor in solid matrices, I. Renge, A. Müller and U.P. Wild 271 (2001) 191
- Photophysical characterization of pyromethene dyes in solid matrices of acrylic copolymers, A. Bergmann, W. Holzer, R. Stark, H. Gratz, A. Penzkofer, F. Amat-Guerri, A. Costela, I. García-Moreno and R. Sastre 271 (2001) 201
- Nonlinear responses (incl. optical)*
- Chain flexibility and nonlinear optical properties in polyenes within a two-state (VB-CT) model, S. Sugliani, M. Del Zoppo, G. Zerbi and C.-F. Shu 271 (2001) 127
- Dispersion of the first molecular hyperpolarizability of charge-transfer chromophores studied by hyper-Rayleigh scattering, J.N. Woodford, C.H. Wang and A.K.-Y. Jen 271 (2001) 137
- Multiphoton phenomena*
- Study on multiphoton processes in intense laser fields using the quadratic anharmonic Lie algebraic hamiltonian of diatomic molecule, Y. Dai, D. Dai and S.-I. Ding 271 (2001) 71
- Photoionization detection of  $\text{CF}_2$  radicals resulting from the IR multiple-photon dissociation of  $\text{CF}_2\text{HCl}$  molecules in a molecular beam, V.N. Lokhman, D.D. Ogurok and E.A. Ryabov 271 (2001) 357
- Tunneling*
- Tunneling splittings in vibrational spectra of non-rigid molecules. X. Reaction path Hamiltonian as zero-order approximation, V.A. Benderskii, E.V. Vetoshkin and H.P. Trommsdorff 271 (2001) 165

*Thermodynamic and transport properties*

Phase behaviors of smectic-A liquid crystal/linear polymer systems, D.K. Yoon and Y.C. Bae

271 (2001) 183

*Critical behavior and phase transitions*

Mass transfer processes induced by inhomogeneous photo-polymerisation in a multicomponent medium, R. Caputo, A.V. Sukhov, N.V. Tabirian, C. Umeton and R.F. Ushakov

271 (2001) 323



